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Resonant Soft X-ray Scattering Study of Chain Ordering in High-Tc superconductor YBCO

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Beamline(s): X1B

Introduction: Resonant soft x-ray scattering (RSXS) is a new synchrotron-based experimental technique that combines both modern spectroscopy and scattering methods. RSXS can selectively measure the ordering phenomena associated with specific elements and orbitals. Particularly, it can directly study the charge/orbital ordering in 3d and 4f systems, where strong correlations and rich ordering phenomena are found to be related to Cu3d, Mn3d, O2p orbitals, etc. The oxygen chain ordering in high temperature superconductors has been observed by conventional hard x-ray scattering [1]. However, it is indirect, and instead of ordered Cu-O chains, it rather measures the displacement of the heavy elements induced by the ordering. On the other hand, RSXS can give direct information of chain ordering and the related electronic structures.

Methods and Materials: The $YBa_2Cu_3O_{6.5}$ single crystal was grown using the flux method, and detwinned under pressure, so that more than 90% of the chains are along the (010) direction. It was subsequently annealed at 40°C for two weeks so that the empty (with one oxygen atom missing) and full Cu-O chains are ordered in a superstructure of a period of 2a (a being the lattice constant). The RSXS experiments were performed in the five-circle diffractometer on the X1B undulator line at the National Synchrotron Light Source. It operates in a vacuum of $2*10^{-10}$mbar for scattering soft x-rays. A channeltron detector is used to detect the scattered photons, and x-ray absorption data were measured with this system as well [2].

Results: As shown in the left panel of Figure 1, momentum transfer is scanned along the (H,0,0) direction. A resonant enhancement of the superstructure (1/2,0,0) Bragg peak corresponding to the chain ordering is observed at the Cu $L_{2,3}$ edge. When E//ac, this enhancement is 58 times stronger at the CuL_3 edge than off resonance (middle panel). In addition, this enhancement is found to change with the azimuthal angle, decreasing by ~30% after rotating the sample by 90 degrees about (100) (right panel) .

Conclusions: Resonant enhancement of the superstructure Bragg peak is observed. The polarization dependence of the Bragg peak intensity at resonance indicates that the chain $Cu3d_{y^2-z^2}$ and $Cu3d_{3z^2-r^2}$ orbitals are mixed significantly, consistent with the low symmetry of the Cu-O rhombus of the chain.

References:

[1] N. H. Andersen *et al.* "Superstructure formation and the structure phase diagram of $YBa_2Cu_3O_{6+x}$ ", Physica C, **317-318**, 259 (1999)

[2] P. Abbamonte *et al.* "A Structural Probe of the Doped Holes in Cuprate Superconductors", Science, **297**, 581 (2002)

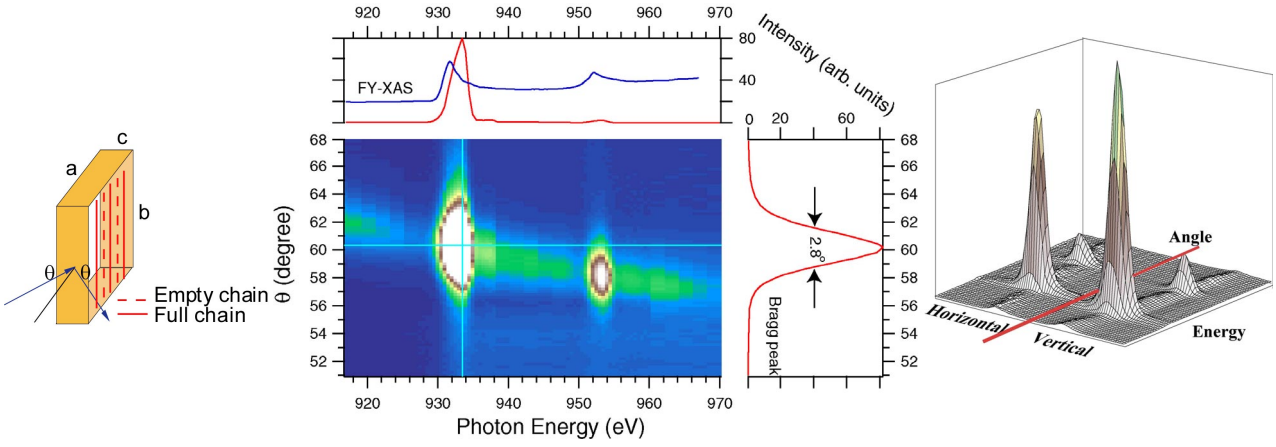

Figure 1. Left panel: illustration of the scattering geometry. Middle panel: the scattering intensity as a function of angle and photon energy, top and right curves are intensities along indicated cuts. Right panel: polarization dependence of the scattering intensity, vertical geometry is for E//ac (same as in the left and middle panel); horizontal geometry is for E//ab, where the sample is rotated by 90 degrees about the (100) direction.